CHE221

SIMULATION LAB 3

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Aim of report:

In this experiment, we explore the atomistic foundation of entropy by simulating energy equilibration between two chambers containing atoms in different energy states. Initially, all atoms in the left chamber are in an excited state, while those in the right chamber remain in the ground state. As energy exchange occurs through a diathermal wall, we analyze the system's progression toward equilibrium.

Introductory Theory

Entropy is a measure of disorder in a system and is maximized when energy is evenly distributed. At the microscopic level, entropy is related to the number of possible arrangements of particles and their energy states. The second law of thermodynamics states that an isolated system tends to evolve toward a state of maximum entropy.

•Energy Exchange and Equilibration: When two systems are allowed to exchange energy, they move toward a state where their energy distribution is uniform, increasing entropy.

•Microstates and Macrostates: A system's macrostate is defined by observable properties like temperature and pressure, while the microstate describes the specific arrangement of particles. More microstates corresponding to a macrostate imply higher entropy.

•Randomized Energy Distribution: Given sufficient time and random exchanges of energy, a system will naturally evolve toward the most probable configuration, which corresponds to thermodynamic equilibrium.

Methodology:

Part1:Create a matrix

N=5;

Construct a binary matrix where the left part contains all 1s and the right part contains all 0s.

Output:

A =

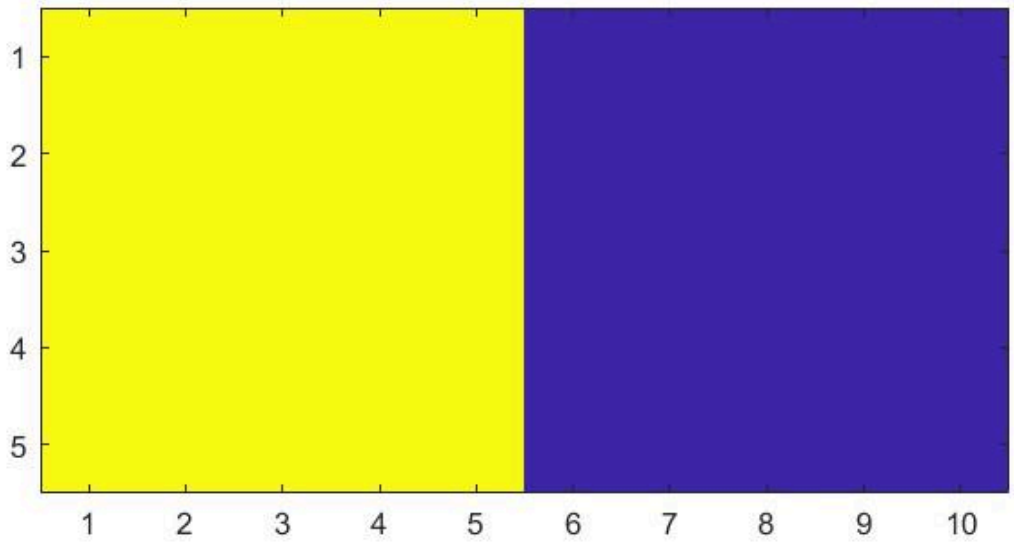
1	1	1	1	1	1	0	0	0	0	0	0
1	1	1	1	1	1	0	0	0	0	0	0
1	1	1	1	1	1	0	0	0	0	0	0

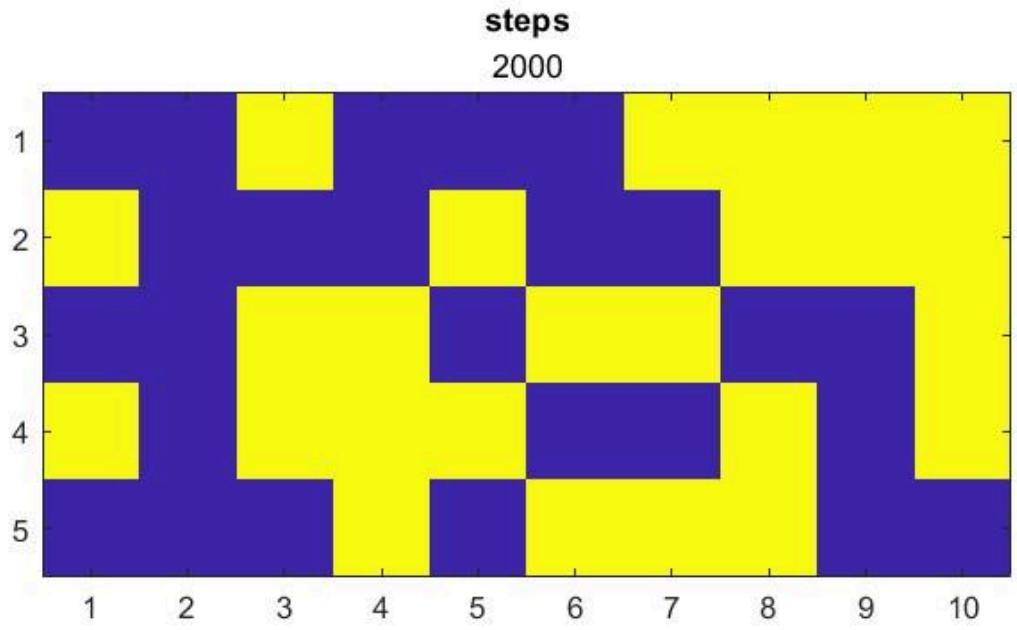
```
     1     1     1     1     1     1     0     0     0     0     0     0
     1     1     1     1     1     1     0     0     0     0     0     0
```

Part2:Function to swap atoms

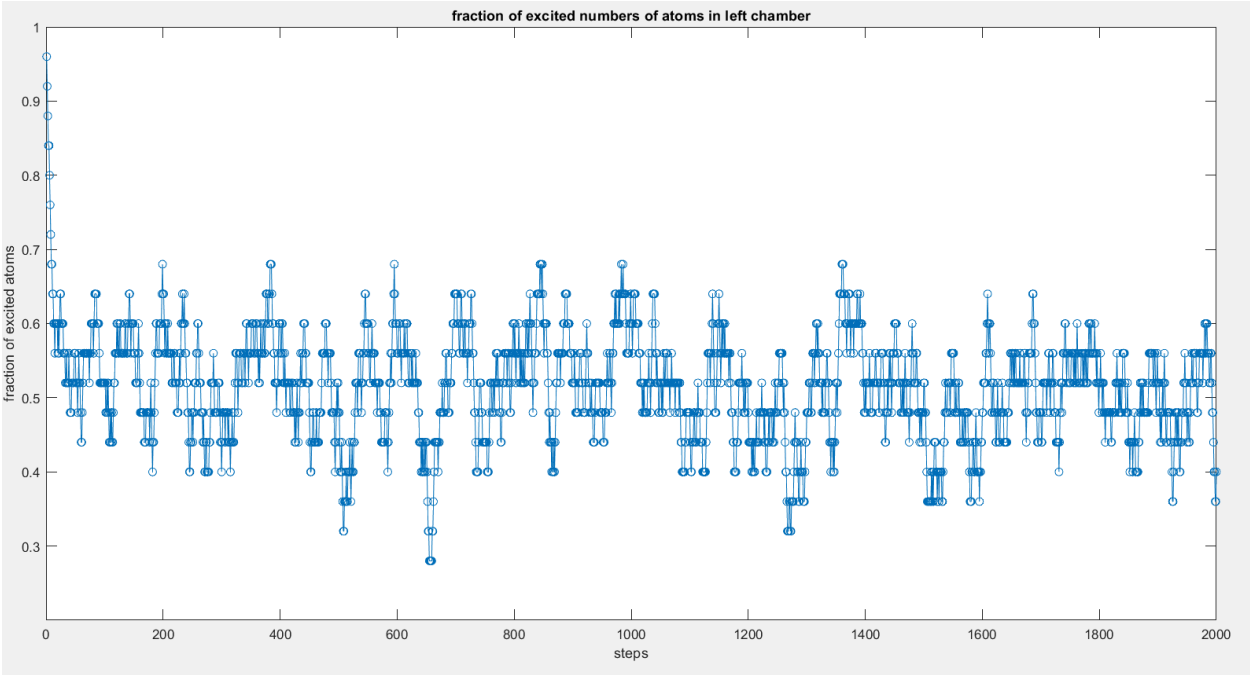
```
A=
     1     1     1     1     0     1     0     1     1     1
     1     1     0     0     0     1     1     0     0     0
     0     1     1     1     0     1     0     0     1     1
     0     0     1     1     0     0     0     0     1     0
     0     0     1     0     0     1     0     1     0     1
```

Part3:Modeling system evolution after walls are made diathermal

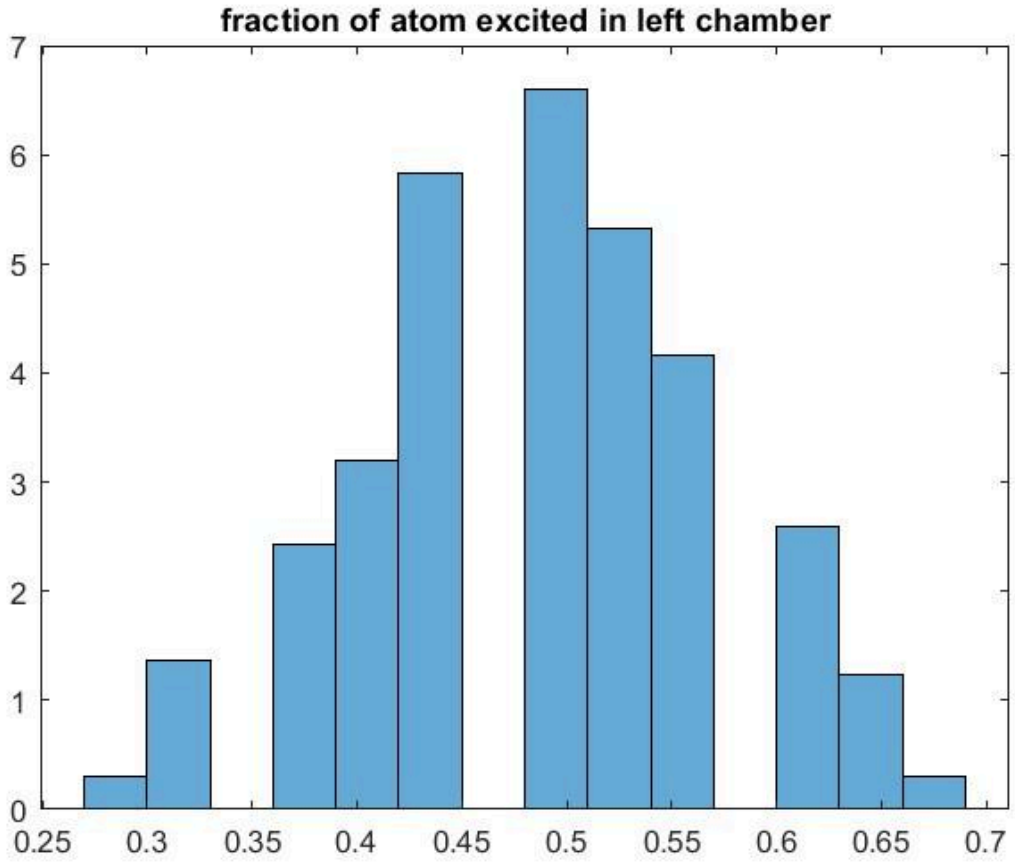



steps
2000
1
2
3
4
5
1
2
3
4
5
6
7
8
9
10

Part4:Collecting and plotting system statistics

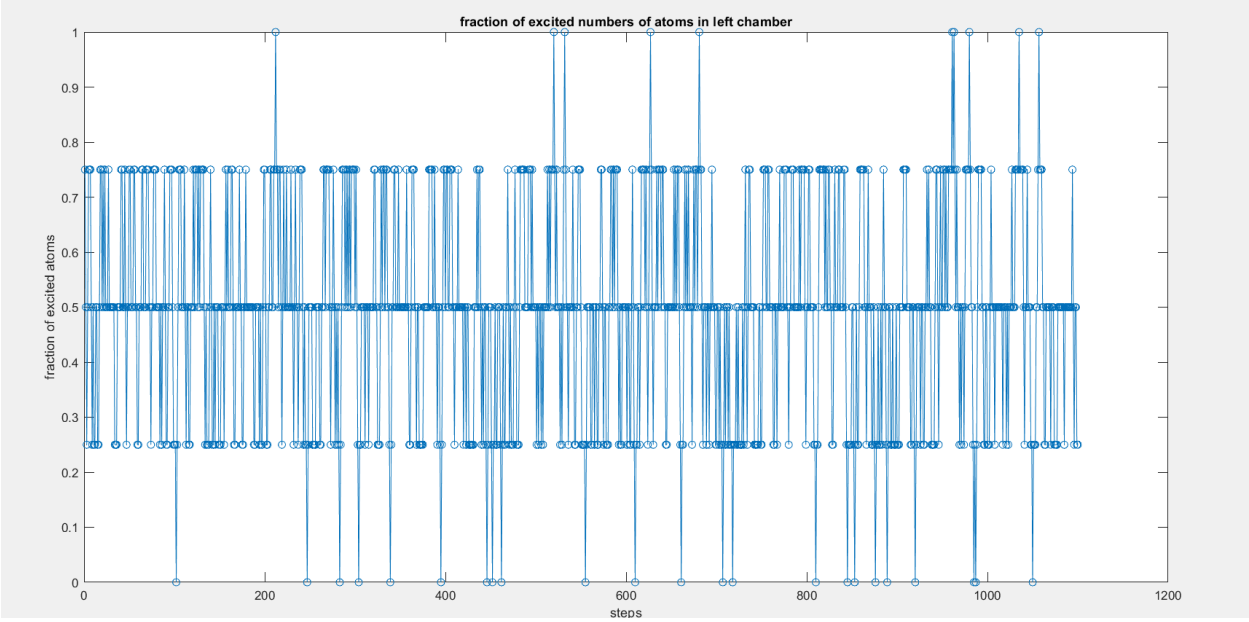


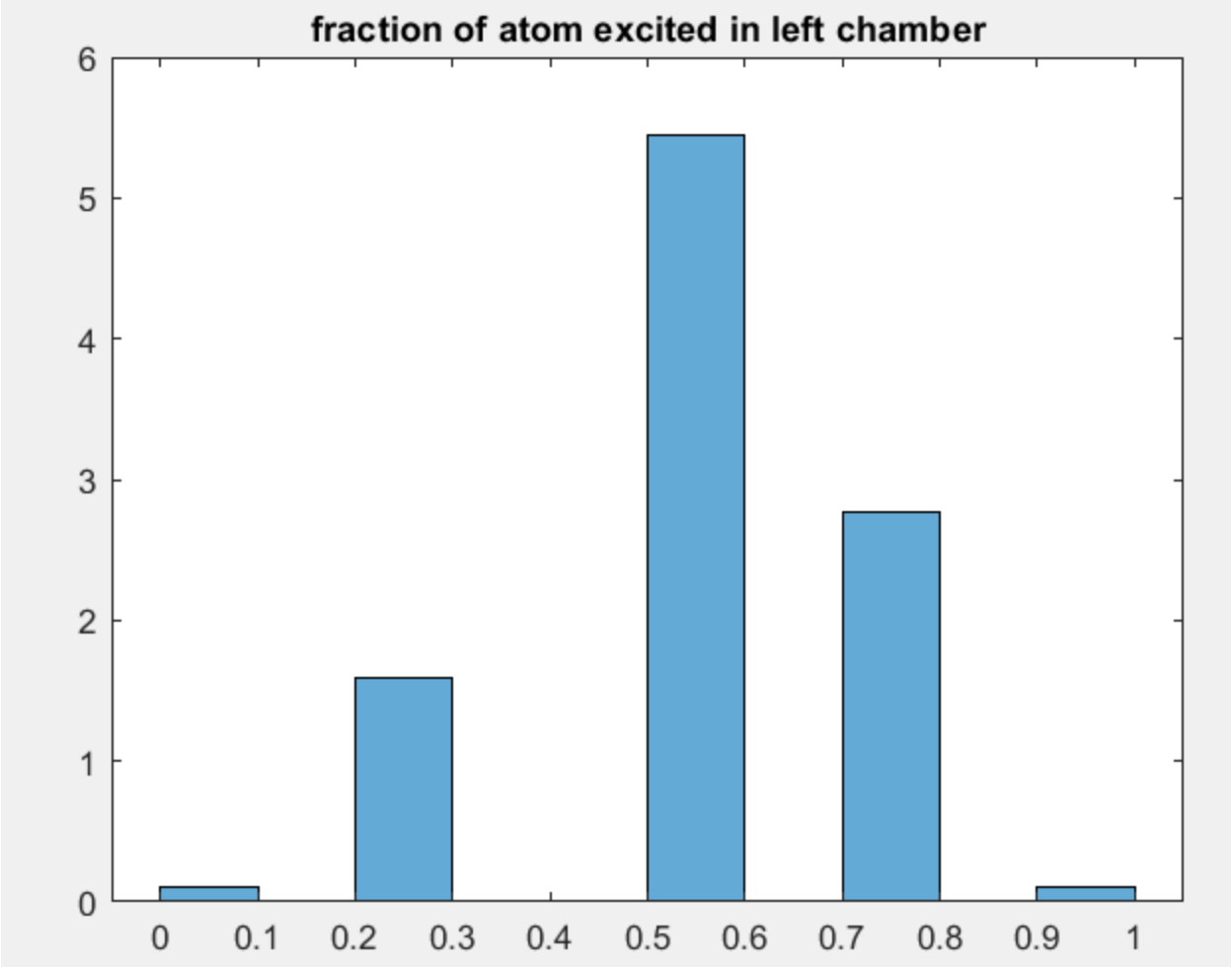
Part5:Plotting system evolution



Part6:Probing the effect of system and size
mean=0.5085
variance=0.0156

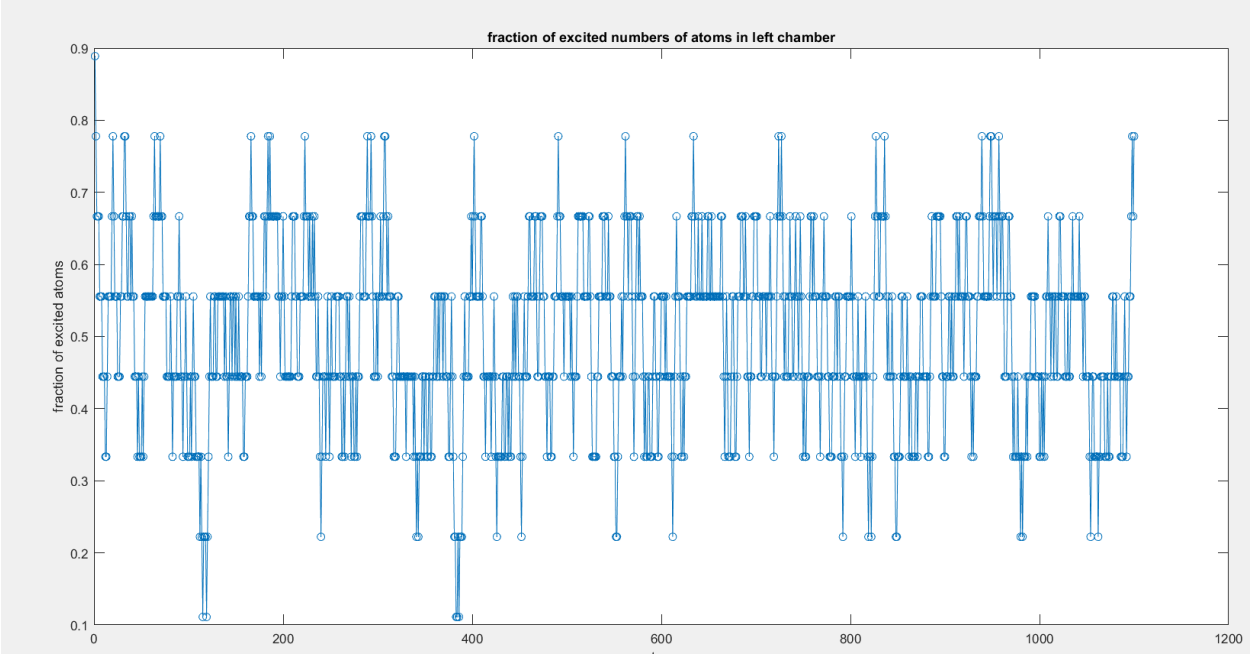
For N=2


fraction of excited numbers of atoms in left chamber
fraction of excited atoms
steps
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
200
400
600
800
1000
1200

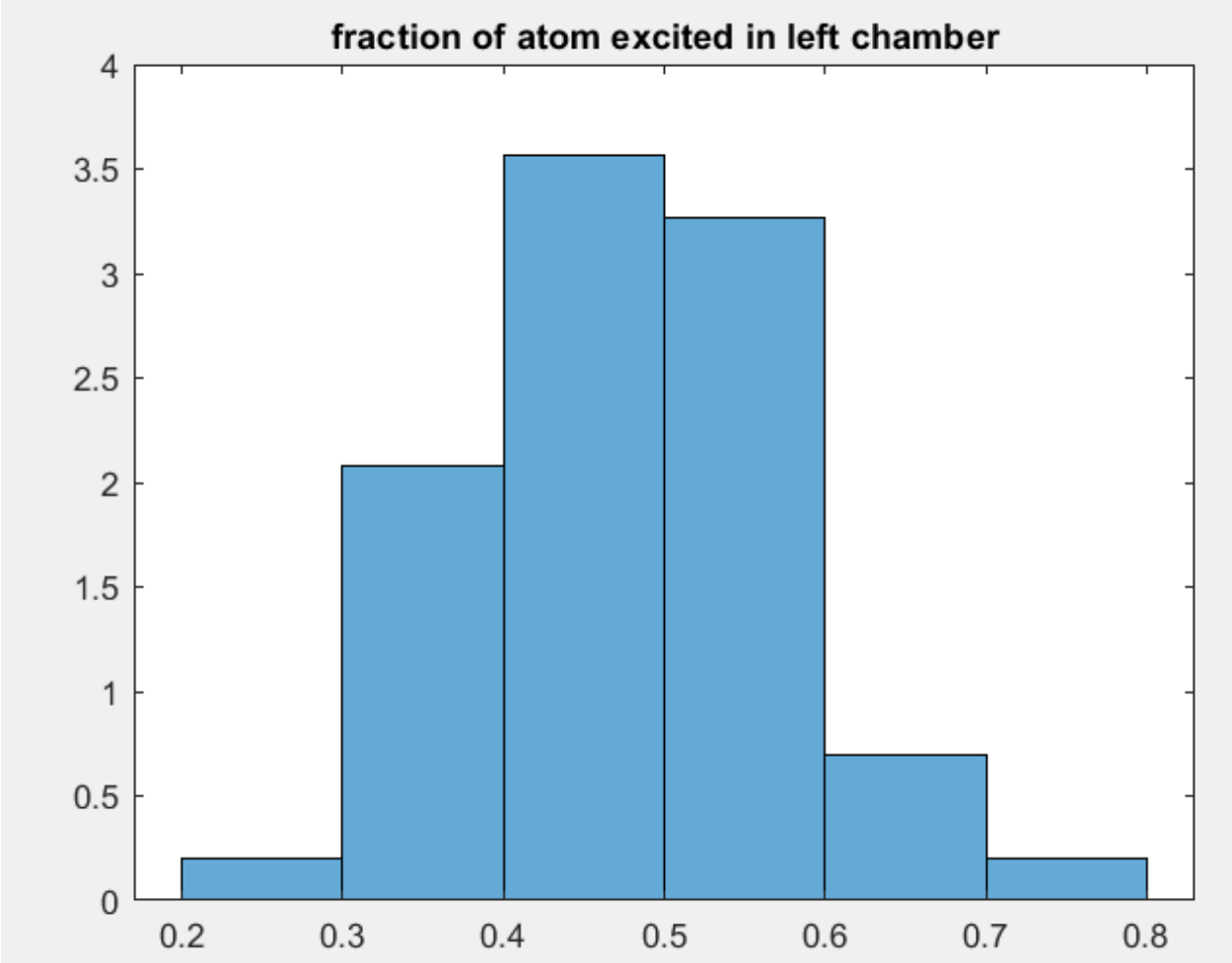


mean= 0.4968
variance= 0.0351

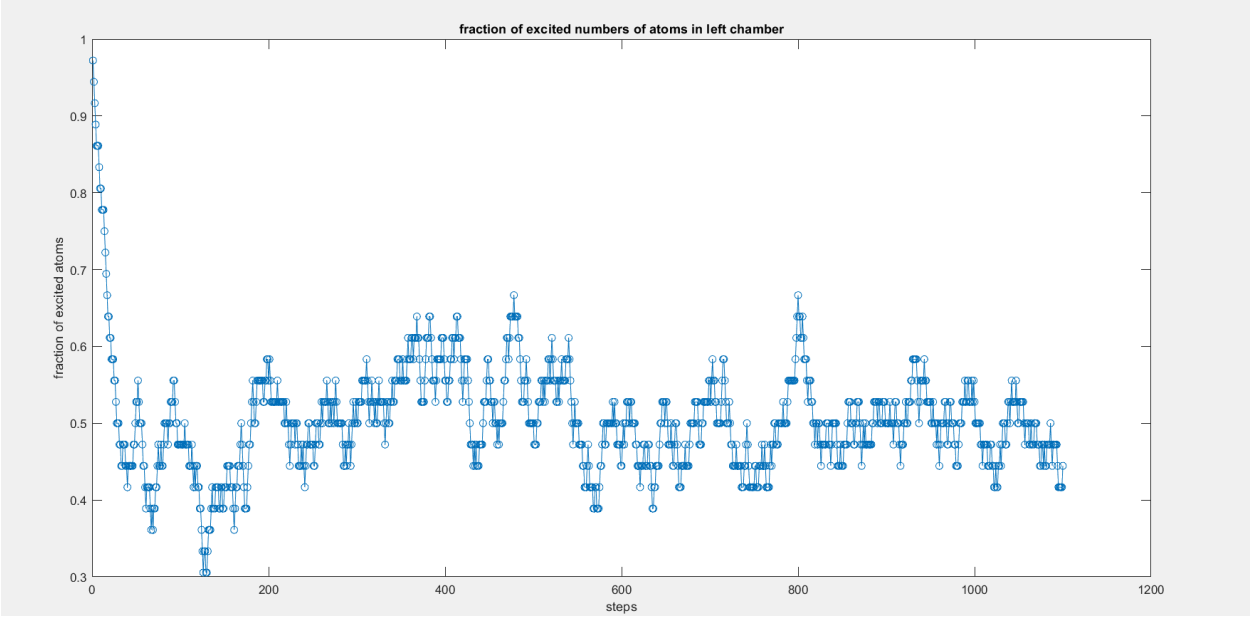
For N=3

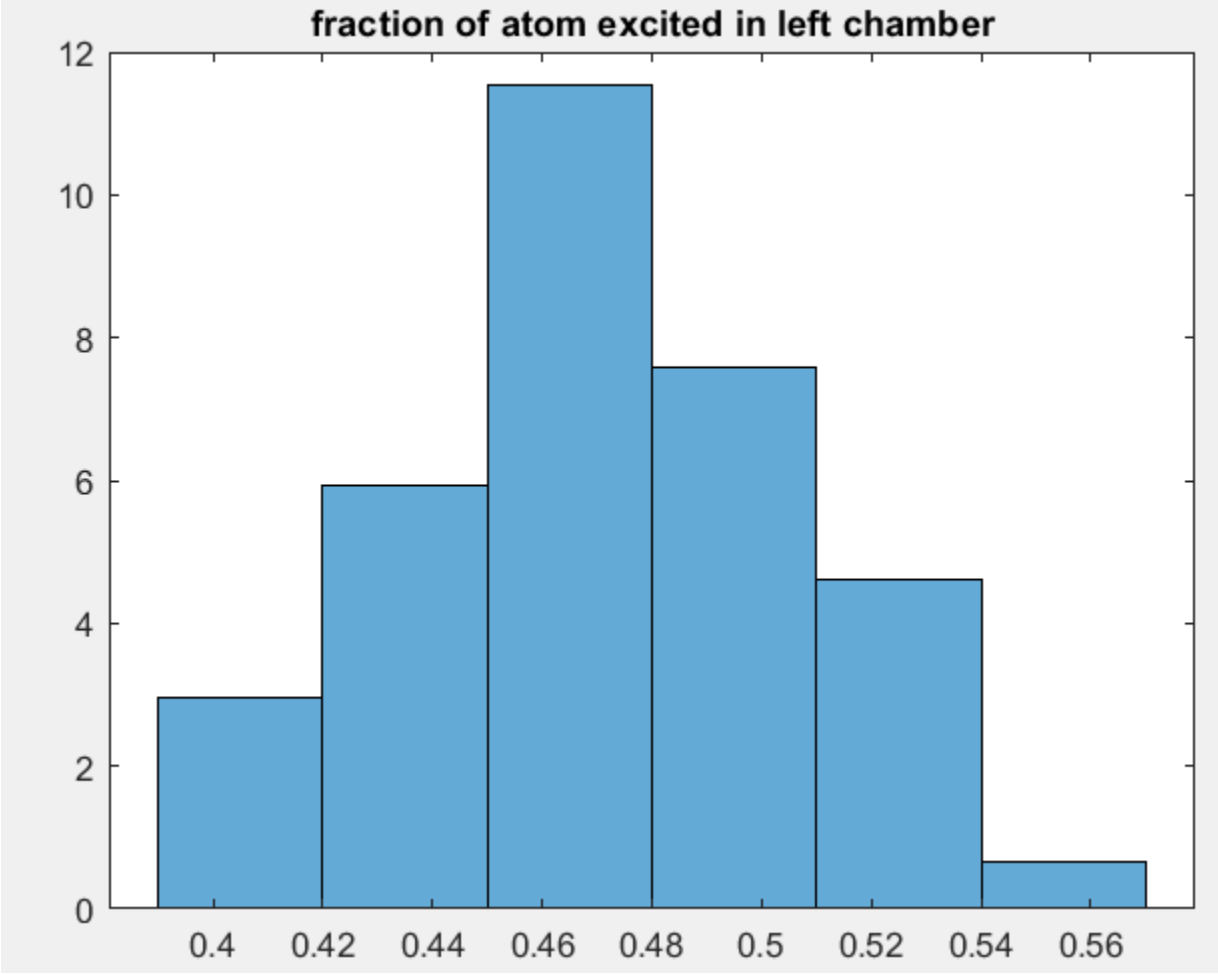


mean=0.4938
variance=0.0159


fraction of atom excited in left chamber
4
3.5
3
2.5
2
1.5
1
0.5
0
0.2
0.3
0.4
0.5
0.6
0.7
0.8

For N=6


fraction of excited numbers of atoms in left chamber
fraction of excited atoms
steps
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0
200
400
600
800
1000
1200


fraction of atom excited in left chamber
12
10
8
6
4
2
0
0.4
0.42
0.44
0.46
0.48
0.5
0.52
0.54
0.56

mean=0.5087
variance=0.0045

Comparison of mean and variance for different N:

N	Mean	Variance
5	0.5085	0.0156
2	0.4968	0.0351
3	0.4938	0.0159
6	0.5087	0.0045

Appendix:

```
clc
clear all
close all
%DEFINE THE MATRIX
N=5;
A=[ones(N),zeros(N)];
figure
imagesc(A);
axis equal tight;
% Pre-define array to record the number of 1s in the left N x N block at
% each step.It records the number of atoms in excited state in left chamber
leftCount = zeros(2000, 1);
plotinterval=1;
fractions=zeros(2000,1);
for i=1:2000
   %B=A;
   A=randomswaps(A);
   leftCount(i)=sum(sum(A(:,1:N)));
   fractions(i)=leftCount(i)/25;

   if mod(i,plotinterval)==0
       imagesc(A);
       axis equal tight
       title('steps',i)
       drawnow
   end
end
%%evolution of the fraction of atoms in
%%the excited state in the left chamber as a function of simulation step
%%number
figure
x=linspace(1,1100,1100);
plot(fractions,'-o');
title('fraction of excited numbers of atoms in left chamber');
xlabel('steps');
ylabel('fraction of excited atoms');
%%histogram
figure
bin=30;
histogram(leftCount(1000:end)/N^2,'Normalization','pdf');
title('fraction of atom excited in left chamber');
%%part 6
%%mean and variance
mean=mean(fractions);
disp(mean);
variance=var(fractions);
disp(variance);
```

RANDOM FUNCTION

```
%% Function to swap indices randomly
function swapped_matrix = randomswaps(M)
%%% Input: a binary matrix M
%%% Output: randomly swap a 1 and 0 in the binary matrix and output the
%%% generated matrix
       % Randomly select an index with entry 1 and then randomly select
       % another index with entry 0.
       % return the swapped matrix
       % Hint: Use find() and randi()
       % return the swapped matrix
x1=find(M==1);
sz1=length(x1);
x2=find(M==0);
sz2=length(x2);
r1=x1(randi(sz1));
r2=x2(randi(sz2));
temp=M(r1);
M(r1)=M(r2);
M(r2)=temp;
swapped_matrix = M;
end
```

Conclusion

This simulation effectively demonstrates entropy-driven energy redistribution at the atomistic level. We observe that as the system evolves, energy tends to spread evenly between chambers, confirming the second law of thermodynamics. Increasing the system size reduces fluctuations, making the equilibrium state more stable.